

IDEAS: A General Purpose Software Package for Simulating Neutron Scattering Instruments

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Introduction

In order to take advantage of the higher neutron flux that new neutron sources will provide, it is essential to develop novel instrumentation. The increasing complexity of neutron scattering instruments and the stringent requirement for efficient use of the available neutrons make it necessary to understand in great detail the compromises inherent in a particular instrument design. While analytical calculations give important insights into the design of an instrument, a detailed evaluation of the instrument performance often goes well beyond what can be calculated analytically. Monte Carlo ray-tracing methods, long recognized as a powerful technique for modeling general radiation transport, are ideally suited to simulation of non-analytic aspects of neutron scattering transport problems and thus design of modern neutron scattering instrumentation. In Monte Carlo ray-tracing simulation, random samplings of the initial state (position, velocity, polarization, and emission time) of a neutron ensemble are repeatedly carried out. The intensity and state of an ensemble are then modified by ray-tracing the neutron trajectories through the instrument.

A comprehensive Monte Carlo simulation package can be used not only for evaluating instrument performance, but also for designing experiments, analyzing experimental results, and training new users of neutron scattering instruments. A modular approach, in which a neutron optical component is represented by a self-contained subroutine or function call, is a natural way of conducting the simulation and allows great flexibility in setting up different instruments and incorporating new components. The main difficulty with developing a general-purpose simulation package lies in the effective management of all of the possible configurations and components that can be used for a particular instrument or experiment. Furthermore, the software must be easy to set up and run so that the users can focus on the outcomes of the simulation, rather than the semantics or details its operation.

IDEAS (Instrument Design and Experiment Assessment Suite) has been designed with these challenges in mind [1]. The simulation engine is written in C++ and runs on Windows platforms. The pre-compiled modules are loaded dynamically at run time, allowing rapid prototyping of an

instrument or experiment. An integrated user interface reduces the work required to construct or change an instrument setup to virtually the click of a button. IDEAS has adopted standard specifications for both the neutron parameters and the subroutine interface structure. This not only ensures the smooth passage of data between the modules, but also guarantees the reusability of existing modules. In addition, users can readily incorporate their own modules coded in C or Fortran.

IDEAS has been applied to instrumentation projects at SNS, ANL, HFIR, HMI, FRM II, and BNL. Specifically, it has been extensively used in the design of the SNS Magnetism Reflectometer [2], the SNS Engineering Diffractometer VULCAN [3,4], and the Neutron Optics Test Station at HFIR [5]. The IDEAS development team also helped to organize a Monte Carlo round robin study [6], comparing the simulation of a model triple-axis spectrometer using various simulation packages. The software and manual are available for download at <http://www.sns.anl.gov>. In the sections below, we shall provide further details on using the software and writing codes for new instrument components. First, however, let us revisit the basis of Monte Carlo simulation for neutron scattering instruments.

Basis of Monte Carlo simulation

The state of a neutron is characterized by $q = (\vec{r}, \vec{v}, \vec{s}, t)$, where the arguments in order are position, velocity, polarization, and time-of-flight (relative to a pre-defined laboratory time). In the initial state (at emission from the moderator), $q_0 = (\vec{r}_o, \vec{v}_o, 0, t_o)$. An instrument component transforms q_0 to state q and changes the intensity of the neutron ensemble. In scattering experiments, the measurable quantity is the number of neutrons counted by a detector. The quantity of interest in most simulations is therefore the intensity at a detector, which is given by the integral,

$$I = \int^{\delta t} dt \int^{\delta \lambda} d\lambda \int^{\delta \Omega} d\Omega \int^A d^2\vec{r} \cdot P(q_0) \cdot \Phi(q_0), \quad (1)$$

where $P(q_0)$ is the transmission function that gives the probability of a neutron recorded by the detector having an initial state q_0 , and $\Phi(q_0)$ is the moderator brilliance (usually given

in the unit of n/sec/Å/ster/cm²). Thus, the simulation problem is essentially reduced to the computation of a multi-dimensional integral, for which the Monte Carlo method is well suited. The basic theorem of Monte Carlo integration estimates the integral of a function f over a multi-dimensional volume V by [7],

$$\int f(x) \cdot dV \approx V \langle f \rangle \pm V \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{M}} \quad (2)$$

where M is the number of sampling points within the volume V , and

$$\langle f \rangle \equiv \frac{1}{M} \sum_{i=1}^M f(x_i) \quad \langle f^2 \rangle \equiv \frac{1}{M} \sum_{i=1}^M f^2(x_i). \quad (3)$$

The second term in Eq. (2) is the standard deviation of the estimated integral. In Eq. (1), the Monte Carlo samplings of the initial neutron state parameters are done within an emission time range δt , the area of the moderator A , a neutron wavelength range $\delta \lambda$, and the solid angle $\delta \Omega$. It follows,

$$I = \frac{1}{M} \sum_{i=1}^M P(q_0) \cdot \Phi(q_0) \cdot [\delta t \cdot A \cdot \delta \lambda \cdot \delta \Omega]. \quad (4)$$

Because an instrument contains many components, $P(q_0)$ usually consists of a series of transmission functions, most of which are quite complex and can only be computed numerically. The computations are carried out along the beam path one component after the other. Modifying the state of a neutron and the intensity of an ensemble within a component is often straightforward so long as the underlining physics is well understood. Additional Monte Carlo sampling will be necessary for components where the state of the neutron is decided by a random selection process. Such components include vanadium, powder samples, and mosaic crystals. Various approaches for simulating mosaic crystals and a vanadium sample have been discussed in detail in Ref. [6].

IDEAS has been designed to carry out either transmission studies or absolute flux calculations for instruments at spallation or reactor sources. Many instrument components are available. Optical components include neutron guides, choppers, slits, and collimators; sample modules include mosaic crystals, focusing monochromators, thin-films, powder samples, vanadium, and inelastic scattering samples. Polarized components include polarizers/analyzers and spin-flippers. In addition, IDEAS is capable of carrying out simulations with multiple beam paths.

Using IDEAS

In IDEAS, instrument components are embedded in self-contained, pre-compiled subroutine modules. A user interface, as shown in Figure 1, is used to arrange these modules in sequence to form an instrument. The sophisticated inte-

gration details discussed above, while forming the basis of the simulation, are hidden.

The right-most panel (INSTRUMENT) in Figure 1 lists the modules that constitute the instrument being studied. Beginning with a neutron source, the components are listed sequentially in the order they are placed along the beam path. The left-most panel shows the user-created folders and the middle panel (COMPONENT) shows the content in the highlighted folder. Each of the user-created folders provides convenient storage for a collection of customized instrument components. In Figure 1, the “TOF Mag. Refl.” folder lists, for example, the components commonly found in a time-of-flight magnetism reflectometer.

The first step in setting up an instrument is to draw a schematic diagram that identifies the origins of the *local* coordinates of each component along the beam path. In IDEAS, each component uses its own coordinates. The origin at the incoming side of a component (e.g., the entry point of a neutron guide) is specified relative to the origin at the outgoing side of the previous component (e.g., the exit point of a guide). A translation or rotation module moves the origin downstream to its new location and orientation. The use of local coordinates allows each instrument component be coded in its own coordinates. It also reduces the number of conversions between local and global coordinates for the neutron parameters, which costs computing time. The time-of-flight of a neutron is always measured relative to an initial laboratory time. In particular, for a pulsed neutron source, the time-of-flight is measured relative to the beginning of a pulse emitted at the moderator.

Once the instrument layout is decided, putting the list of components in IDEAS is done by simply dragging the relevant modules from the COMPONENT panel to the INSTRUMENT panel. Likewise, the ordering of the instrument components can be rearranged by dragging them up and down the list. Double-clicking a component brings up a window listing the parameters of the component; see the call-out in Figure 1. To change the parameters, simply type the new values.

When the user is satisfied with the setup of the instrument, a click on the “Start” button starts the simulation. The relevant pre-compiled libraries are loaded and the details of the component parameters are passed to the libraries. The simulation loops then start. Each simulation loop begins with a Monte Carlo sampling in a source module that generates the intensity and state of a neutron ensemble within the specified ranges. The intensity and state are then modified sequentially by the list of components subject to the physics of the interaction. The simulation loops will repeat until the pre-set number of samplings is reached or until the user stops the run. Real-time monitoring of the results is available with the data collection module. Machine-speed computation is achieved by directly calling the ray-tracing subroutines.

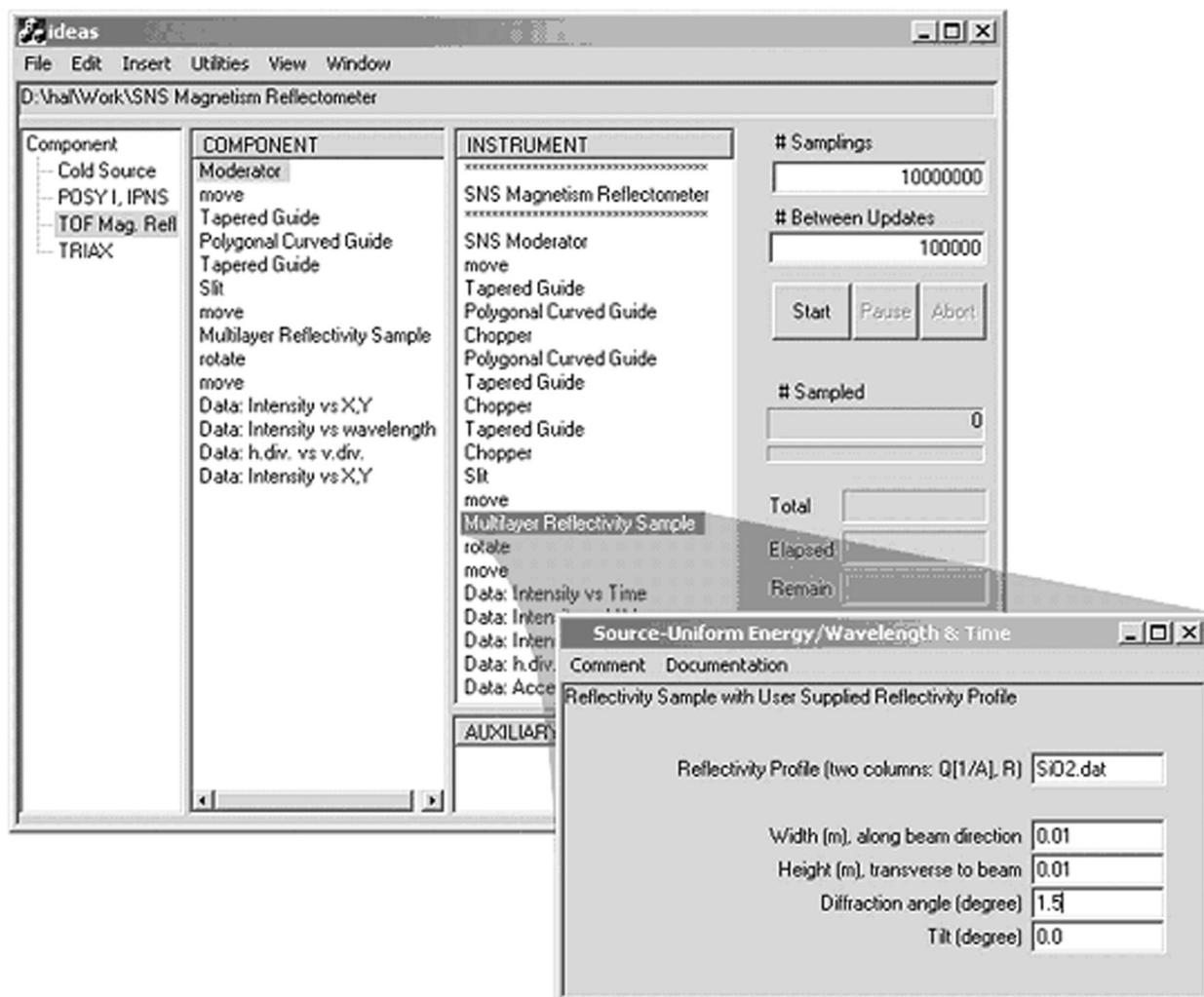


Figure 1. User interface for setting up an instrument profile in IDEAS. Details are explained in the text. Double clicking an instrument component brings up a standard user interface where parameters for the component are specified.

Writing a new module

A basic suite of components is provided with IDEAS. However, an instrument often has its own unique components. IDEAS has been designed to include new components, either through source code or pre-compiled dynamic-link-libraries (DLL). The codes for an instrument component are written in standard C or FORTRAN. To allow flexibility in coding while ensuring a smooth passage of data between the components, IDEAS adopts a *single* convention for code writing, i.e., the arguments for all subroutines are five pointers each pointing to an object with a defined data structure. Details of these five objects, which include the neutron state parameters and the component specifications, are explained in the IDEAS manual. A program is included with IDEAS to

streamline the work from compiling the code (user can also compile the codes themselves) to putting the compiled library in the right place. The program also automatically generates a user interface (see Figure 1) from a list of component parameters. In addition to the ray-tracing subroutine, other *optional* subroutines may be used with IDEAS to carry out additional tasks, such as real-time analysis of the simulation results.

An example: The SNS magnetism reflectometer

IDEAS has been extensively used in the design of the SNS Magnetism Reflectometer [2], which is schematically shown in Figure 3. The neutron guide system that transports thermal neutrons from the moderator to the sample position

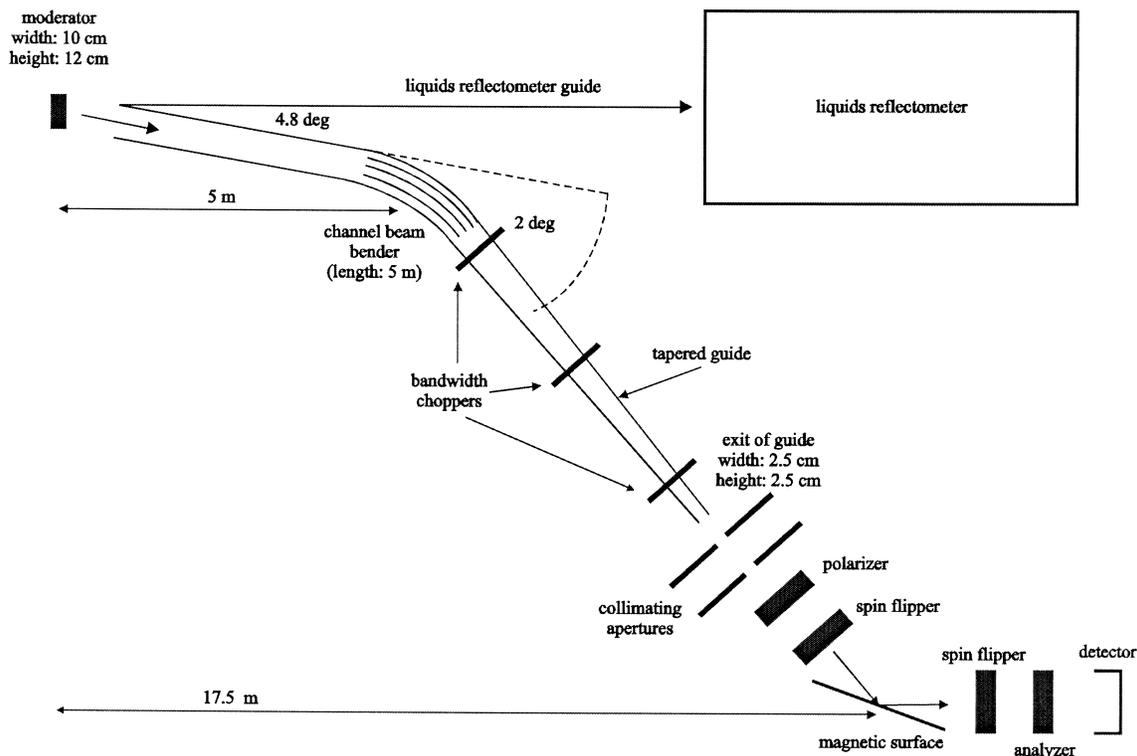


Figure 2. Schematic diagram of the SNS Magnetism Reflectometer.

consists of a series of tapered and polygonal curved guides. The use of a curved guide keeps the sample position out of the line-of-sight of the moderator, greatly reducing the high-energy neutron background. Optimization was carried out to maximize the thermal neutron intensity while minimizing the high-energy background [8]. The design constraints are (a) getting out of the line-of-sight at 10.5 m from the moderator, and (b) making the sample to moderator distance at least 17.5 m. To evaluate the performance of the optimized instrument design, a reflectivity experiment was simulated using the reflectivity profile of a 10 Å SiO₂ thin film on a silicon substrate as the sample. To assess the capabilities of the SNS reflectometers in resolving data from monolayer films, we assume a 25 x 25 mm² sample area, an incident angle of 20°, a wavelength-resolution $\Delta\lambda/\lambda = 10\%$ (achieved by an appropriate time-binning of the data), and an angular resolution of $\Delta\theta/\theta = 10\%$ (achieved by using a pair of slits that are 0.5 m apart). The SNS coupled liquid hydrogen moderator profile was calculated separately [9] using the MCNP software.

Figure 3a shows the reflectivity profile generated from the simulation with the theoretical reflectivity curve (assuming an ideal resolution function) superimposed. As can be seen, the coarse resolution setting is still reasonable since it does not significantly reduce the resolution for the reflectivity

measurements on this monolayer film. Because we carried out an absolute flux calculation, we can estimate the count-rate on the detector that will be achieved for the 10 Å SiO₂ film. As shown in Figure 3b, data points that represent reflectivity intensities of some 10⁻⁹ can still be measured with a very reasonable count-rate of the order of 0.2 counts/sec. With proper shielding, the background count-rate is expected to be at least a factor of five smaller. Note that the pulsed operation of the instrument will allow simultaneous data collection with a bandwidth of 3.5 Å. For example, a band from 6.1 Å to 2.6 Å can be used as indicated in the figure. Typically, a reasonable counting statistic is achieved when 100 counts are accumulated for each data point; the marked region can be therefore measured with a data collection time of 8 min. The completion of the reflectivity scan (data collection in the low Q region) will require less time.

Summary

An overview of IDEAS, a Monte Carlo ray-tracing software package for simulation of neutron scattering instrumentation, has been given. We have first explained the basis of the Monte Carlo simulation approach. This was followed by a brief description of how to set up and run a simulation in IDEAS and a guideline for writing codes for additional in-

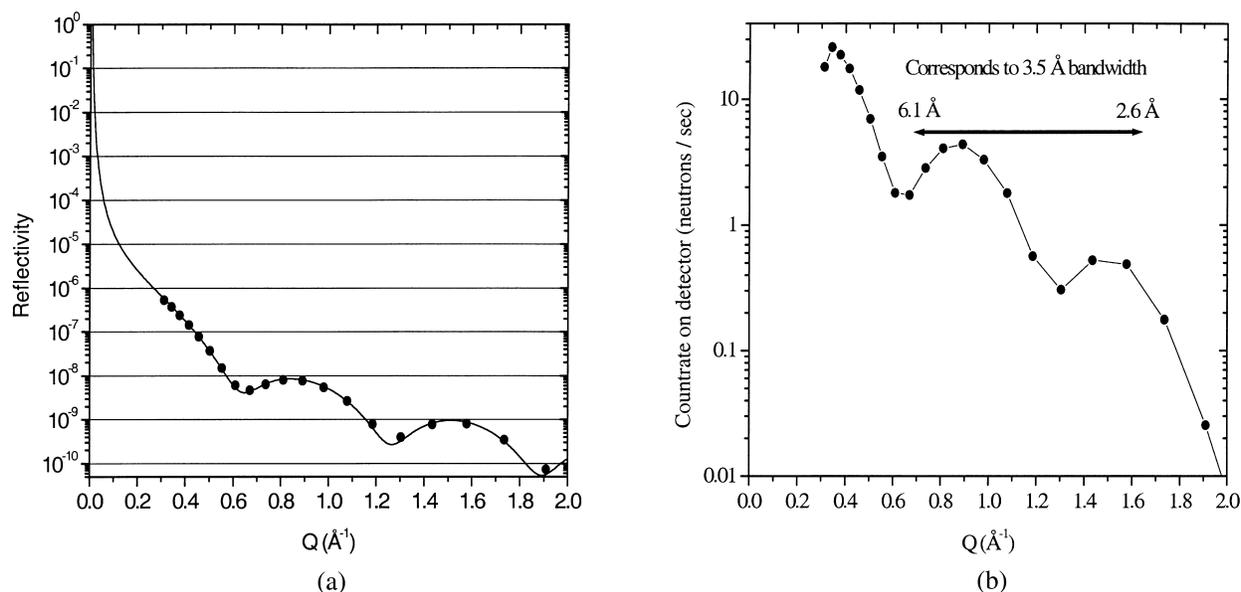


Figure 3. Results of an absolute flux calculation for a reflectivity measurement on a 10 Å SiO₂ film on a Si substrate. (a) Reflectivity profile. The data points are from the simulation and the solid line is the theoretical reflectivity. (b) Estimated count rate on the detector. The simulation suggests that the marked region from 6.1 Å to 2.6 Å (at 10^{-9} level) can be measured in 8 minutes.

strument components. Finally, we have provided a case study using the simulation of the SNS Magnetism Reflectometer. IDEAS is a versatile simulation package developed for ease of use and incorporation of new instrument components. We expect that IDEAS will be a valuable tool for evaluating new neutron scattering instruments, in the design of scattering experiments, and for the education of new users.

IDEAS will be maintained by the authors and volunteers. A basic suite of components is provided with the program. However, users are welcome to write new component modules to meet their own simulation needs. Components with proven test results and documentation will be included in the official component library and available to general users.

Acknowledgments

The authors wish to thank J. L. Robertson for his contribution in the early stage of this work, R. K. Crawford for helpful discussions, F. Klose for providing the simulation information of the SNS Magnetism Reflectometer, and E. B. Iverson for critical reading of the manuscript. IDEAS was conceived and partially developed with the support of a Laboratory Directed Research and Development Program from Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

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